

Anaerobic degradation of Dithiopyr in four soils

Report: MRID 50092201. Cooper, J. 2016. [¹⁴C]-Dithiopyr: Route and Rate of Degradation in Four Soils under Anaerobic Conditions at 20°C. Unpublished study performed by Battelle UK Ltd., Chelmsford, Essex, United Kingdom; sponsored and submitted by Dow AgroSciences LLC, Indianapolis, Indiana. Laboratory Study ID: YR/15/003. Dow AgroSciences Study ID: 150624. Study initiated July 31, 2015, and completed- October 18, 2016; experimental start and end dates were not reported (p. 3). Final report issued October 18, 2016.

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Statements: The study was conducted according to OECD and UK GLP standards (p. 3). Signed and dated Data Confidentiality, GLP, and Quality Assurance statements were provided (pp. 2-5). A certification of the authenticity of the report is included in the Quality Assurance statement (pp. 4-5).


Classification: This study is classified as **supplemental**. Although pE+pH values were less than 12, the detection of dissolved oxygen in some post-flooded sampling intervals suggested that test systems did not entirely remain in anaerobic conditions during the test period. Pesticide use history at the two US soil collection sites was not reported, and it was not confirmed that the soils were free of pesticides prior to use.

PC Code: 128994

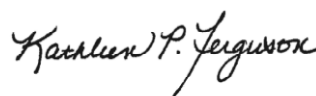
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This Data Evaluation Record may have been altered by the Environmental Fate and Effects Division subsequent to signing by CDM/CSS-Dynamac JV personnel.

EXECUTIVE SUMMARY

The anaerobic transformation of [pyridine-4-¹⁴C]dithiopyr was studied in four soils from North Dakota: a clay loam soil (DU-L-PF; pH 6.2) from North Dakota; a silt loam soil (pH 6.1) from Iowa, a clay loam soil (Hareby; pH 7.5) from the UK, and a sandy loam soil (pH 7.5) from the UK. The soils were treated at 4.66 mg a.i./kg, equivalent to a field rate of 1.75 kg a.i./ha, and incubated for 30 days in darkness at 20°C with a soil moisture content of pF 2, then were flooded, placed

under a nitrogen atmosphere, and incubated an additional 120 days. Duplicate samples (two entire flasks) were collected for analysis at each sampling interval.

In the water column of the flooded DU-L-PF clay loam soil system, standard redox potentials, oxygen saturation and pH were -138 to +130 mV, 0-4%, and 7.10-8.07, respectively, with standard redox potentials in the soil of -62 to +89 mV. In the water column of the silt loam soil system, standard redox potentials, oxygen saturation and pH were +2 to +173 mV, 0-3%, and 6.44-8.23, respectively, with standard redox potentials in the soil of -10 to +88 mV. In the water column of the Hareby clay loam soil system, standard redox potentials, oxygen saturation and pH were -44 to +103 mV, 0-4%, and 8.39-9.24, respectively, with standard redox potentials in the soil of -165 to +13 mV. In the water column of the sandy loam soil system, standard redox potentials, oxygen saturation and pH were -35 to +91 mV, 0-4%, and 8.49-9.33, respectively, with standard redox potentials in the soil of -94 to +47 mV. The flooded test systems were suboxic at all intervals postflooding. The soils were viable at study initiation and termination.

In the DU-L-PF clay loam soil system, overall mass balances averaged $100.06 \pm 2.70\%$ (range 93.80-105.26%) of the applied. In the silt loam soil system, overall mass balances averaged $100.05 \pm 2.74\%$ (range 95.74-103.72%). In the Hareby clay loam soil system, overall mass balances averaged $100.44 \pm 2.24\%$ (range 97.03-104.59%). In the sandy loam soil system, overall mass balances averaged $100.06 \pm 2.51\%$ (range 95.68-104.37%). Recoveries in all systems were within guideline criteria (90-110%).

Observed DT₅₀ values, calculated half-lives, and information on transformation products are listed in **Table 1**. Dithiopyr dissipated from the water plus sediment with SFO DT₅₀ values of 682 days in the DU-L-PF clay loam soil system, 2,166 days in the silt loam soil system, 795 days in the Hareby clay loam soil system, and 1,861 days in the sandy loam soil system. The degradation SFO DT₅₀ value (using volatile-adjusted EPTC concentrations) was 6,439 days in the Hareby clay loam soil system; dithiopyr was stable in the other test systems. No transformation products were detected, and two minor transformation products were identified.

In the water from the DU-L-PF clay loam soil system, total residues were a maximum of 2.56% of the applied at 37 days postflooding and decreased to 2.15% at 120 days. In the soil, total extractable radioactivity declined from 99.46% at time 0 to 82.01% at 120 days postflooding. Unextracted radioactivity was a maximum of 10.33% at 15 days posttreatment and decreased to 6.11% at 120 days postflooding. CO₂ and organic volatiles in the ethylene glycol traps totaled <0.1% throughout the study. Organic volatiles in the polyurethane foam plugs, which were identified as dithiopyr, were a maximum of 13.09% at 120 days postflooding.

In the water from the silt loam soil system, total residues were a maximum of 3.93% of the applied at 120 days postflooding. In the soil, total extractable radioactivity declined from 100.35% at time 0 to 82.52% at 120 days postflooding. Unextracted radioactivity was a maximum of 8.11% at 30 days posttreatment and decreased to 7.64% at 120 days postflooding. CO₂ and organic volatiles in the ethylene glycol traps totaled <0.1% throughout the study. Organic volatiles in the polyurethane foam plugs, which were identified as dithiopyr, were a maximum of 11.35% at 120 days postflooding.

In the water from the Hareby clay loam soil system, total residues were a maximum of 4.34% of the applied at 30 days post-flooding and decreased to 3.90% at 120 days. In the soil, total extractable

radioactivity declined from 100.35% at time 0 to 81.07% at 120 days postflooding. Unextracted radioactivity was a maximum of 6.67% at 30 days posttreatment and decreased to 6.27% at 120 days postflooding. CO₂ and organic volatiles in the ethylene glycol traps totaled <0.1% throughout the study. Organic volatiles in the polyurethane foam plugs, which were identified as dithiopyr, were a maximum of 8.77% at 120 days postflooding.

In the water from the sandy loam soil system, total residues were a maximum of 4.35% of the applied at 120 days postflooding. In the soil, total extractable radioactivity declined from 102.29% at time 0 to 91.05% at 120 days postflooding. Unextracted radioactivity was a maximum of 3.51% at 30 days posttreatment and decreased to 1.85% at 120 days postflooding. CO₂ and organic volatiles in the ethylene glycol traps totaled <0.1% throughout the study. Organic volatiles in the polyurethane foam plugs, which were identified as dithiopyr, were a maximum of 9.21% at 120 days postflooding.

Table 1. Results Synopsis: Anaerobic Soil Metabolism of Dithiopyr.

Total System	Observed DT ₅₀ (days)	Calculated Half-life (days) ¹	Model Parameters and Statistics ¹	Transformation Products Common Name (maximum % AR, associated interval) ²	
				Major	Minor
North Dakota USA Clay loam soil (DU- L-PF) (20°C, soil pH 6.2)	Dissipation kinetics ³			Unextracted residues (10.33%, 15 days posttreatment)	CP108329 (2.44%, 7 days postflooding) CP108330 (2.44%, 120 days postflooding) CO ₂ (<0.1%, all intervals)
	>120	682 SFO	C ₀ = 84.9 k = 0.00102 S _C = 63.6 S _{SFO} = 60.2		
	Degradation kinetics ⁴				
	>120	Stable			
Iowa, USA Silt loam soil (20°C, soil pH 6.1)	Dissipation kinetics ³			None	CP108329 (1.55%, 30 days postflooding) CP108330 (1.58%, 120 days postflooding) CO ₂ (<0.1%, all intervals)
	>270	2,166 SFO	C ₀ = 84 k = 0.000322 S _C = 50 S _{SFO} = 38.9		
	Degradation kinetics ⁴				
	>120	Stable			
UK Clay loam soil (Hareby) (20°C, soil pH 7.5)	Dissipation kinetics ³			None	CP108329 (1.57%, 120 days postflooding) CP108330 (2.79%, 120 days postflooding) CO ₂ (<0.1%, all intervals)
	>120	795 SFO	C ₀ = 90.2 k = 0.000872 S _C = 51.8 S _{SFO} = 40		
	Degradation kinetics ⁴				
	>120	6,439 SFO	C ₀ = 90.8 k = 0.000108 S _C = 51.7 S _{SFO} = 40.3		
UK Sandy loam soil (20°C, soil pH 7.5)	Dissipation kinetics ³			None	CP108329 (1.40%, 120 days postflooding) CP108330 (1.66%, 120 days postflooding) CO ₂ (<0.1%, all intervals)
	>120	1,861 SFO	C ₀ = 91 k = 0.000372 S _C = 148 S _{SFO} = 116		
	Degradation kinetics ⁴				
	>120	Stable			

¹ Calculated half-lives, model parameters, and kinetics models in accordance with the NAFTA kinetics guidance (USEPA, 2012); Single First Order (SFO). Data from 30 days posttreatment was 0 days postflooding.

² AR means “applied radioactivity”.

³ Based on dithiopyr in the soil:water.

⁴ Based on dithiopyr in the total system (includes volatilized dithiopyr).

I. Materials And Methods

A. Materials:

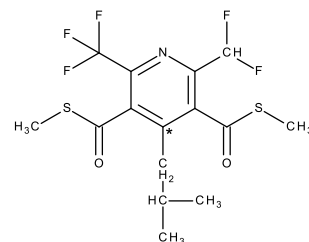
1. Test Material [Pyridine-4-¹⁴C]dithiopyr (p. 18; Figure 1, p. 51)

Specific activity: 57.1 mCi/mMol

Radiochemical purity: 96.74%

Chemical purity: Not reported

Batch No.: DE3-124733-47



Solubility in water: 1.4 mg/L at 20°C (p. 17)

2. Reference Compounds: The following standards were used in the analysis (Table 2).

Table 2. Reference Compounds.

Applicant's Code Name	Chemical Name	Purity (%)	Batch No.
Dithiopyr	S,S'-Dimethyl-2-(difluoromethyl)-4-isobutyl-6-(trifluoromethyl)-pyridine-3,5-dicarbothioate	--	E1442-54
Diacid (RH-133972)	2-(Difluoromethyl)-4-isobutyl-6-(trifluoromethyl)pyridine-3,5-dicarboxylic acid	--	CMT-4352C
CP108329	6-(Difluoromethyl)-4-(2-methylpropyl)-5-(methylthio)carbonyl-2-(trifluoromethyl)-3-pyridinecarboxylic acid	--	PIT-9101-2665-A
CP108330	2-(Difluoromethyl)-4-(2-methylpropyl)-5-(methylthio)carbonyl-6-(trifluoromethyl)-3-pyridinecarboxylic acid	--	PIT-9101-2666-A

Data obtained from p. 18 and Figure 1, pp. 51-52, in the study report. Chemical names from DER Attachment 1.

-- = not reported.

3. Soil: Soil collection and characterization are summarized in Table 3 and Table 4, respectively.

Table 3. Description of Soil Collection and Storage.

Description	DU-L-PF	Iowa	Hareby	Longwoods
Geographic location	Grand Forks, North Dakota	Jackson, Iowa	Site J3, Hareby House, Lincolnshire, UK	Site 12, Longwoods Quarry, Lincolnshire, UK
Site description	Not reported		Grassy corner between arable field and woodland	Unworked former arable land
Soil series	Not reported			
Pesticide use history at the collection site	Unknown		None for "some years"	None for 16 years
Collection date	July 27, 2015	July 28, 2015	July 23, 2015	July 27, 2015
Collection procedures	By shovel	By shovel	By spade	By spade
Sampling depth	0-6 inches	0-6 inches	4-10 cm	5-20 cm
Storage	Stored according to Standard ISO/DISS 10381-6 Part 6			

Description	DU-L-PF	Iowa	Hareby	Longwoods
Storage length	Not reported. Soils were preincubated under study conditions for 6 days prior to use.			
Soil preparation	Sieved (2 mm)			

Data obtained from pp. 18-19; Tables 1-2, pp. 35-36; and Appendix C, p. 87, of the study report.

Table 4. Properties of the Soils.

Property	DU-L-PF	Iowa	Hareby	Longwoods
Soil Texture	Clay loam	Silt loam	Clay loam	Sandy loam
% Sand	33	15	41	69
% Silt	38	64	21	19
% Clay	29	21	38	12
pH (in 0.01M CaCl ₂)	6.2	6.1	7.5	7.5
Organic carbon (%)	6.9	1.9	2.4	2.0
Organic matter (%) ¹	11.9	3.3	4.1	3.4
Cation Exchange Capacity (meq/100 g)	22.6	12.2	13.9	11.9
CaCO ₃ equivalence (%)	Not reported			
Soil Moisture Content (%)				
0.1 bar (2.0 pF)	51.9	42.2	25.8	16.6
0.33 bar (2.5 pF)	42.3	29.1	22.3	12.1
Bulk density (g/cm ³ , disturbed)	0.87	1.00	1.10	1.24
Microbial Biomass (mg C/kg soil)				
At start of aerobic phase	739 ± 26	167 ± 7	241 ± 19	571 ± 18
At termination of anaerobic phase	443 ± 19	184 ± 8	405 ± 5	121 ± 11
Soil taxonomic classification	Not reported			

Data obtained from Table 1, p. 35, of the study report. The soil textures were confirmed using USDA-NRCS technical support tools.

¹ Calculated by the reviewer as: organic matter (%) = organic carbon (%) x 1.72.

B. STUDY DESIGN

1. Experimental Conditions: (Summarized in Table 5).

Table 5. Experimental Design.

Property	Details
Duration of the test (days)	150 days (30 days aerobic, 120 days anaerobic)
Soil condition (Air dried/fresh)	Soils were preincubated under study conditions for 6 days prior to use.
Soil (g/replicate)	100 g (dry wt)
Water (mL/replicate)	120-140 mL
Application rates	
Nominal	4.483 mg a.i./kg, equivalent to a field rate of 1.68 kg a.i./ha
Actual	0.466 mg a.i./100 g
Control conditions (if used)	Sterile controls were not used.
Number of Replicates	
Controls (if used)	Sterile controls were not used.
Treatment	For each soil, duplicate samples (two entire flasks) were collected at each sampling interval.

Property	Details
Test apparatus	
Type/material/volume	The test system consisted of straight-sided flasks (volume not reported) containing moist soil (100 g dry wt) that were incubated under study conditions for 6 days prior to treatment. After treatment, the flasks were attached to individual flow-through volatile trapping systems. On Day 30 posttreatment, the soil was flooded with deoxygenated water and the sample flasks were flushed with nitrogen prior to being reattached to the volatile trapping system. Samples were kept in the dark in a constant temperature incubator. The test system is illustrated in Figure 4, p. 55.
Details of traps for CO ₂ and other volatiles (if any)	Humidified CO ₂ -free air or nitrogen gas were continuously drawn through a sample (flow rate not reported), then through a polyurethane foam plug, one tube of ethylene glycol, and two tubes of 2M KOH solution. The trapping apparatus is illustrated in Figure 4, p. 55.
If no traps were used, is the system closed/open?	Volatile traps were used.
Identity and concentration of co-solvent	Acetonitrile, <0.1% (v:w)
Test Material:	
Volume of the test solution used/treatment	225 µL/100 g
Application method	Applied evenly to the soil surface using a positive displacement pipette. The flasks were then gently agitated.
Is the co-solvent evaporated?	Yes
Any indication of the test material adsorbing to the walls of the test apparatus?	None
Experimental conditions:	
Temperature (°C)	20 ± 2°C
Continuous darkness	Yes
Moisture content	pF 2.0 during aerobic incubation
Moisture maintenance method	Soil was remoistened once during the aerobic phase of the study; water added when necessary during the anaerobic phase.
Other details (if any)	None

Data obtained from pp. 18-21; Table 2, p. 36; and Figure 4, p. 55, of the study report.

2. Sampling During Study Period: (Details summarized in Table 6).

Table 6. Sampling During Study Period.

Criteria	Details
Sampling intervals	0, 15 and 30 days posttreatment 7, 14, 30, 70, and 120 days postflooding
Sampling method	For each soil, duplicate samples (two entire flasks) were collected at each sampling interval.
Method of collection of CO ₂ and organic volatile compounds	Volatile traps were collected at each sampling interval.
Sampling intervals/times for:	

Criteria	Details
Sterility check (if used)	Sterile controls were not used.
Moisture content	Soil was remoistened once during the aerobic phase of the study; water added when necessary during the anaerobic phase.
Redox potential in water layer	At 1, 7, 14, 30, 70, and 121 days postflooding
Dissolved oxygen in water layer	
pH in water layer	
Redox potential in soil	
pH in soil	
Sample storage before analysis	The water and soil were separated at the time of collection. Samples were analyzed within 15 days of collection. Samples were frozen (<-15°C) when not in use, except subsamples of the traps were stored at room temperature after the initial assay.
Other observation (if any)	None.

Data obtained from pp. 21, 24; Tables 2-3, pp. 36-37; and Table 5, p. 39, of the study report.

3. Analytical Procedures

Extraction/Clean Up/Concentration Methods: When present, the water layer was decanted from the soil (p. 21). Aliquots of the water were analyzed using LSC. The remaining water was combined with the soil extracts prior to HPLC analysis.

The soil was transferred to plastic bottles and extracted three times with acetonitrile:water (80:20, v:v) and twice with acetonitrile:formic acid (100:0.1, v:v) by shaking at room temperature (20 minutes/extraction, p. 22). After each extraction, the mixture was centrifuged and the supernatant decanted. Like extracts were combined and aliquots analyzed using LSC. Aliquots of the water and the acetonitrile:water extracts were combined and analyzed using HPLC. Aliquots of the acetonitrile:formic acid extracts were analyzed using HPLC. Solutions were not concentrated prior to analysis because of the possibility of volatilization.

Select samples (Day 30 posttreatment, Days 14-120) of the extracted DU-L-PF clay loam soil were further extracted twice with tetrahydrofuran and twice with cyclohexane by shaking at room temperature (20 minutes/extraction; pp. 22-23). After each extraction, the mixture was centrifuged and the supernatant decanted. Like extracts were combined and aliquots analyzed using LSC. Aliquots of the tetrahydrofuran extracts were analyzed using HPLC.

Determination of Unextracted Residues: The undried extracted soils were homogenized and analyzed for total radioactivity by LSC following combustion (pp. 22-23).

Determination of Volatile Residues: The foam plugs were extracted with organic solvent, and the extracts were analyzed using LSC; residues were characterized by HPLC (pp. 21, 24). The ethylene glycol and NaOH trapping solutions were analyzed using LSC. The presence of CO₂ in the NaOH solutions was not confirmed.

Total Radioactivity Measurement: Total [¹⁴C]residues were determined by summing the concentrations of residues measured in the water, soil extracts, extracted soil, and trapping solutions (Tables 6-9, pp. 40-43).

Derivatization Method: A derivatization method was not described.

Identification and Quantification of Parent and Transformation Compounds: Aliquots of the water, soil extracts, and foam plug extracts were analyzed by HPLC using a Kromasil 100 C18 analytical column eluted with a gradient mobile phase of (A) water = 0.1% formic acid (v:v) and (B) acetonitrile + 0.1% formic acid (v:v; p. 24; Table 4, p. 38). The eluate was monitored with radioactivity and UV detectors. Chromatographic peak retention times were compared to those of reference standards. Samples with insufficient radioactivity to detect using HPLC were analyzed by HPLC-TopCount details not provided).

Identification of dithiopyr was confirmed by LC-MS (p. 24).

Detection Limits (LOD, LOQ) for the Parent and Transformation Products: For LSC, the Limit of Detection (LOD) was 1.5x background and the Limits of Quantification (LOQ) were 0.01% of the applied for the soil extracts, 0.006% for the polyurethane foam plus, 0.000013% for the ethanolamine, and 0.00000078% for the KOH (Appendix F, pp. 106-107). For HPLC, the LOQ was 0.07% for all solutions (Appendix G, p. 109).

II. Results and Discussion

A. Data

Study results including total mass balances and distribution of radioactivity are presented in **Tables 6-9**. In the water column of the flooded DU-L-PF clay loam soil system, standard redox potentials, oxygen saturation and pH were -138 to +130 mV, 0-4%, and 7.10-8.07, respectively, with standard redox potentials in the soil of -62 to +89 mV (Table 5, p. 39). In the water column of the Iowa silt loam soil system, standard redox potentials, oxygen saturation and pH were +2 to +173 mV, 0-3%, and 6.44-8.23, respectively, with standard redox potentials in the soil of -10 to +88 mV. In the water column of the Hareby clay loam soil system, standard redox potentials, oxygen saturation and pH were -44 to +103 mV, 0-4%, and 8.39-9.24, respectively, with standard redox potentials in the soil of -165 to +13 mV. In the water column of the sandy loam soil system, standard redox potentials, oxygen saturation and pH were -35 to +91 mV, 0-4%, and 8.49-9.33, respectively, with standard redox potentials in the soil of -94 to +47 mV. The flooded test systems were suboxic at all intervals postflooding.

Soils were viable at study initiation and at termination (Table 1, p. 35).

B. Mass Balance

In the DU-L-PF clay loam soil system, overall mass balances averaged $100.06 \pm 2.70\%$ (range 93.80-105.26%) of the applied (Table 6, p. 40). In the silt loam soil system, overall mass balances averaged $100.05 \pm 2.74\%$ (range 95.74-103.72%; Table 7, p. 41). In the Hareby clay loam soil system, overall mass balances averaged $100.44 \pm 2.24\%$ (range 97.03-104.59%; Table 8, p. 42). In the sandy loam soil system, overall mass balances averaged $100.06 \pm 2.51\%$ (range 95.68-104.37%; Table 9, p. 43). Recoveries in all systems were within guideline criteria (90-110%).

C. Unextracted and Extractable Residues

In the water from the DU-L-PF clay loam soil system, total residues were a maximum of 2.56% of the applied at 37 days postflooding and decreased to 2.15% at 120 days (Table 6, p. 40). In the soil, total extractable radioactivity declined from 99.46% at time 0 to 82.01% at 120 days postflooding. Unextracted radioactivity was a maximum of 10.33% at 15 days posttreatment and decreased to 6.11% at 120 days postflooding.

In the water from the silt loam soil system, total residues were a maximum of 3.93% of the applied at 120 days postflooding (Table 7, p. 41). In the soil, total extractable radioactivity declined from 100.35% at time 0 to 82.52% at 120 days postflooding. Unextracted radioactivity was a maximum of 8.11% at 30 days posttreatment and decreased to 7.64% at 120 days postflooding.

In the water from the Hareby clay loam soil system, total residues were a maximum of 4.34% of the applied at 30 days postflooding and decreased to 3.90% at 120 days (Table 8, p. 42). In the soil, total extractable radioactivity declined from 100.35% at time 0 to 81.07% at 120 days postflooding. Unextracted radioactivity was a maximum of 6.67% at 30 days posttreatment and decreased to 6.27% at 120 days postflooding.

In the water from the sandy loam soil system, total residues were a maximum of 4.35% of the applied at 120 days postflooding (Table 9, p. 43). In the soil, total extractable radioactivity declined from 102.29% at time 0 to 91.05% at 120 days postflooding. Unextracted radioactivity was a maximum of 3.51% at 30 days posttreatment and decreased to 1.85% at 120 days postflooding.

D. Volatilization

In all test systems, CO₂ and organic volatiles in the ethylene glycol traps totaled <0.1% of the applied throughout the study (Tables 6-9, pp. 40-43). Organic volatiles in the polyurethane foam plugs, which were identified as dithiopyr, were maximums of 13.09% of the applied in the DU-L-PF clay loam soil system, 11.35% in the silt loam soil system, 8.77% in the Hareby clay loam soil system and 9.21% in the sandy loam soil system at 120 days postflooding.

Table 7a. Anaerobic transformation of dithiopyr, expressed as a percentage of the applied radioactivity, in DU-L-PF clay loam soil.

Sampling Interval (days)	Aerobic						Anaerobic (days after flooding)									
	0		15		30 (0)		7		14		30		70		120	
Replicate Number	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B
Dithiopyr in water/soil ¹	95.69	91.72	88.01	82.48	87.43	86.80	83.48	84.62	79.94	85.34	81.53	82.46	74.67	79.14	74.66	78.70
Total Dithiopyr	95.69	91.72	89.61	85.37	89.88	89.02	85.62	85.88	83.74	86.59	85.55	89.08	85.72	89.00	87.75	86.67
Volatile-adj EPTC in w+s ²	95.69	91.72	89.56	85.27	89.84	89.03	85.47	85.83	83.52	86.55	85.42	89.15	85.60	89.07	87.96	86.47
CP108329	0.00	0.00	0.67	1.25	1.44	1.49	2.44	1.84	1.75	1.69	1.33	0.95	1.99	0.54	1.52	1.14
CP108330	0.00	0.00	1.05	1.34	1.34	1.60	1.41	1.51	1.50	1.80	1.72	1.50	2.40	1.04	2.44	2.05
Others ³	3.78	1.69	0.43	0.54	0.84	1.58	1.13	1.53	1.50	0.63	0.91	0.66	2.92	1.08	0.88	0.94
Water	--	--	--	--	--	--	2.07	1.87	--	1.97	2.56	2.29	1.31	1.44	2.15	0.93
Extracted residues ⁴	99.46	93.41	91.76	88.50	93.50	93.69	88.54	88.89	94.02	92.60	83.56	85.11	80.91	80.57	77.58	82.01
Unextracted residues	5.80	9.77	6.64	10.33	5.28	5.92	8.83	7.85	4.07	4.03	3.68	4.67	5.45	5.80	5.90	6.11
Total volatile compounds ⁵	0.00	0.00	1.60	2.89	2.45	2.22	2.14	1.26	3.80	1.25	4.02	6.62	11.05	9.86	13.09	7.97
Mass balance	105.26	103.18	100.00	101.73	101.22	101.82	101.58	99.87	101.89	99.84	93.80	98.68	98.71	97.68	98.72	97.03

Data obtained from Table 6, p. 40, and Table 10, p. 44, of the study report.

1 Nonvolatilized dithiopyr calculated as Total Dithiopyr minus Total volatile compounds.

2 Value for test compound in water + sediment adjusted for loss of volatilized test compound using the following equation:

[volatile-adjusted test compound in w+s] = [previous volatile-adjusted test compound in w+s] × exp[(Δvolatile organics - Δtest compound in w+s) ÷ mean test compound in w+s over previous interval]

3 Others is the sum of several minor compounds, none >5% of the applied (Table 10, p. 44).

4 Sum of soil extracts 1-9.

5 Volatile concentrations in the individual traps were not reported. The ethylene glycol or KOH traps contained <0.1% of the applied (Table 6, p. 40).

n.a. = not analyzed.

Table 7b. Anaerobic transformation of dithiopyr, expressed as a percentage of the applied radioactivity, in Iowa silt loam soil.

Sampling Interval (days)	Aerobic						Anaerobic (days after flooding)									
	0		15		30 (0)		7		14		30		70		120	
Replicate Number	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B
Dithiopyr in water/soil ¹	98.11	97.96	92.95	87.16	81.43	85.27	83.06	84.42	85.92	81.90	83.50	81.88	82.91	84.79	77.63	82.07
Total Dithiopyr	98.11	97.96	93.46	90.17	90.92	91.49	89.03	87.76	87.11	87.33	88.51	90.73	90.57	93.22	88.98	90.55
Volatile-adj EPTC in w+s ²	98.11	97.96	93.45	90.05	90.77	91.44	88.70	87.51	86.71	87.06	88.16	90.75	90.37	93.50	88.59	90.56
CP108329	0.00	0.00	1.12	0.59	0.98	0.88	0.94	0.71	1.07	1.23	1.55	0.85	0.66	0.74	1.22	0.00
CP108330	0.00	0.00	0.69	0.72	1.11	1.01	1.12	0.92	0.77	1.35	1.42	1.12	1.22	1.14	1.45	1.58
Others ³	2.01	2.39	0.99	0.81	1.12	1.44	1.15	0.76	0.95	1.76	0.61	0.18	2.12	1.21	1.14	2.57
Water	--	--	--	--	--	--	3.54	3.21	3.19	3.47	3.46	3.46	2.16	2.47	3.93	3.86
Extracted residues ⁴	100.12	100.35	96.28	92.28	84.83	88.73	82.93	83.77	85.71	82.94	83.74	80.74	84.91	85.55	77.79	82.52
Unextracted residues	3.59	3.36	3.82	4.88	6.78	8.11	3.66	5.42	6.27	7.19	5.02	5.11	7.79	5.00	6.21	7.64
Total volatile compounds ⁵	0.00	0.00	0.51	3.01	9.49	6.22	5.97	3.34	1.19	5.43	5.01	8.85	7.66	8.43	11.35	8.48
Mass balance	103.72	103.71	100.61	100.17	101.11	103.06	96.08	95.74	96.36	99.04	97.24	98.16	102.53	101.46	99.28	102.50

Data obtained from Table 7, p. 41, and Table 11, p. 45, of the study report.

1 Nonvolatilized dithiopyr calculated as Total Dithiopyr minus Total volatile compounds.

2 Value for test compound in water + sediment adjusted for loss of volatilized test compound using the following equation:

[volatile-adjusted test compound in w+s] = [previous volatile-adjusted test compound in w+s] × exp[(Δvolatile organics - Δtest compound in w+s) ÷ mean test compound in w+s over previous interval]

3 Others is the sum of several minor compounds, none >5% of the applied (Table 11, p. 45).

4 Sum of soil extracts 1-5.

5 Volatile concentrations in the individual traps were not reported. The ethylene glycol or KOH traps contained <0.1% of the applied (Table 7, p. 41).

n.a. = not analyzed.

Table 7c. Anaerobic transformation of dithiopyr, expressed as a percentage of the applied radioactivity, in Hareby clay loam soil.

Sampling Interval (days)	Aerobic						Anaerobic (days after flooding)									
	0		15		30 (0)		7		14		30		70		120	
Replicate Number	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B
Dithiopyr in water/soil ¹	96.79	98.98	87.32	93.41	91.15	90.03	87.31	87.01	90.13	89.49	89.63	88.40	88.93	83.47	79.34	81.09
Total Dithiopyr	96.79	98.98	90.68	94.04	92.36	91.57	88.13	88.10	90.73	90.27	91.41	91.98	93.98	90.78	88.11	89.17
Volatile-adj EPTC in w+s ²	96.79	98.98	90.57	94.03	92.30	91.53	88.02	88.01	90.64	90.20	91.33	91.95	94.00	90.68	87.66	88.92
CP108329	0.00	0.00	0.64	0.81	1.05	0.83	1.10	0.89	1.06	1.13	1.02	1.50	0.92	0.99	1.57	1.15
CP108330	0.00	0.00	0.68	0.73	1.12	0.99	2.07	1.73	1.32	1.65	1.23	1.09	1.63	1.80	2.79	2.00
Others ³	3.44	1.36	1.92	0.87	0.78	1.04	1.07	0.92	0.96	1.04	0.60	0.24	0.36	1.99	0.74	0.65
Water	--	--	--	--	--	--	2.11	2.78	2.11	2.63	4.34	3.65	3.24	3.15	3.82	3.90
Extracted residues ⁴	100.23	100.35	93.92	96.44	95.31	94.42	90.25	88.86	91.95	91.47	88.13	87.69	88.72	85.17	80.70	81.07
Unextracted residues	3.52	4.24	4.55	5.34	6.06	6.67	5.19	4.29	4.18	5.08	4.02	3.28	3.36	3.90	6.27	5.99
Total volatile compounds ⁵	0.00	0.00	3.36	0.63	1.21	1.54	0.82	1.09	0.60	0.78	1.78	3.58	5.05	7.31	8.77	8.08
Mass balance	103.75	104.59	101.84	102.42	102.58	102.64	98.37	97.03	98.85	99.97	98.27	98.20	100.37	99.53	99.56	99.04

Data obtained from Table 8, p. 42, and Table 12, p. 46, of the study report.

1 Nonvolatilized dithiopyr calculated as Total Dithiopyr minus Total volatile compounds.

2 Value for test compound in water + sediment adjusted for loss of volatilized test compound using the following equation:

[volatile-adjusted test compound in w+s] = [previous volatile-adjusted test compound in w+s] × exp[(Δvolatile organics - Δtest compound in w+s) ÷ mean test compound in w+s over previous interval]

3 Others is the sum of several minor compounds, none >5% of the applied (Table 12, p. 46).

4 Sum of soil extracts 1-5.

5 Volatile concentrations in the individual traps were not reported. The ethylene glycol or KOH traps contained <0.1% of the applied (Table 8, p. 42).

n.a. = not analyzed.

Table 7d. Anaerobic transformation of dithiopyr, expressed as a percentage of the applied radioactivity, in Longwoods sandy loam soil.

Sampling Interval (days)	Aerobic						Anaerobic (days after flooding)									
	0		15		30 (0)		7		14		30		70		120	
Replicate Number	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B
Dithiopyr in water/soil ¹	100.72	98.72	93.32	97.00	96.56	85.61	92.32	89.28	91.19	93.23	91.47	86.63	86.71	86.60	91.25	85.34
Total Dithiopyr	100.72	98.72	93.61	97.17	97.03	87.88	92.91	90.41	91.87	94.82	93.67	92.15	94.88	95.30	95.10	94.55
Volatile-adj EPTC in w+s ²	100.72	98.72	93.60	97.17	97.04	87.77	92.89	90.34	91.85	94.82	93.68	92.04	94.96	95.45	95.19	94.62
CP108329	0.00	0.00	0.70	0.73	0.67	0.70	0.28	0.61	1.27	0.96	0.84	1.03	0.59	0.63	1.40	0.73
CP108330	0.00	0.00	0.62	0.00	0.44	0.95	1.19	0.62	0.68	0.51	1.32	0.50	0.88	1.02	1.48	1.66
Others ³	1.58	3.17	1.77	1.60	0.71	0.96	0.64	0.67	1.39	1.72	0.88	2.25	1.29	0.61	0.65	0.45
Water	--	--	--	--	--	--	1.33	2.39	2.26	2.93	3.06	3.80	3.78	3.55	3.79	4.35
Extracted residues ⁴	102.29	101.88	96.70	99.51	98.85	90.48	93.69	89.92	92.95	95.09	91.52	86.68	85.73	85.36	91.05	84.51
Unextracted residues	2.08	1.89	1.75	2.29	3.25	3.51	1.72	2.24	2.89	2.55	3.13	2.35	2.97	2.36	1.76	1.85
Total volatile compounds ⁵	0.00	0.00	0.29	0.17	0.47	2.27	0.59	1.13	0.68	1.59	2.20	5.52	8.17	8.70	3.85	9.21
Mass balance	104.37	103.77	98.74	101.97	102.57	96.27	97.33	95.68	98.78	102.16	99.91	98.36	100.66	99.97	100.45	99.93

Data obtained from Table 9, p. 43, and Table 13, p. 47, of the study report.

1 Nonvolatilized dithiopyr calculated as Total Dithiopyr minus Total volatile compounds.

2 Value for test compound in water + sediment adjusted for loss of volatilized test compound using the following equation:

[volatile-adjusted test compound in w+s] = [previous volatile-adjusted test compound in w+s] × exp[(Δvolatile organics - Δtest compound in w+s) ÷ mean test compound in w+s over previous interval]

3 Others is the sum of several minor compounds, none >5% of the applied (Table 13, p. 47).

4 Sum of soil extracts 1-5.

5 Volatile concentrations in the individual traps were not reported. The ethylene glycol or KOH traps contained <0.1% of the applied (Table 9, p. 43).

n.a. = not analyzed.

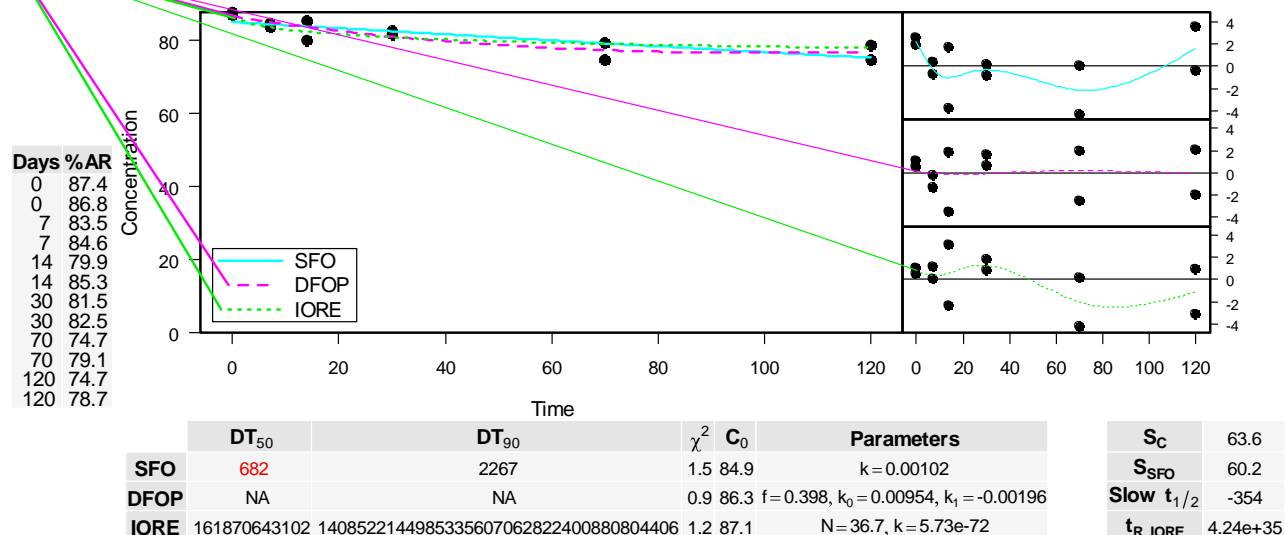
E. Transformation of the Test Compound

Dissipation kinetics (nonvolatilized) and degradation kinetics (volatile-adjusted) of dithiopyr from the test systems during the anaerobic phase of the study are summarized in the following **Figures**, with transformation product information summarized in **Table 8**.

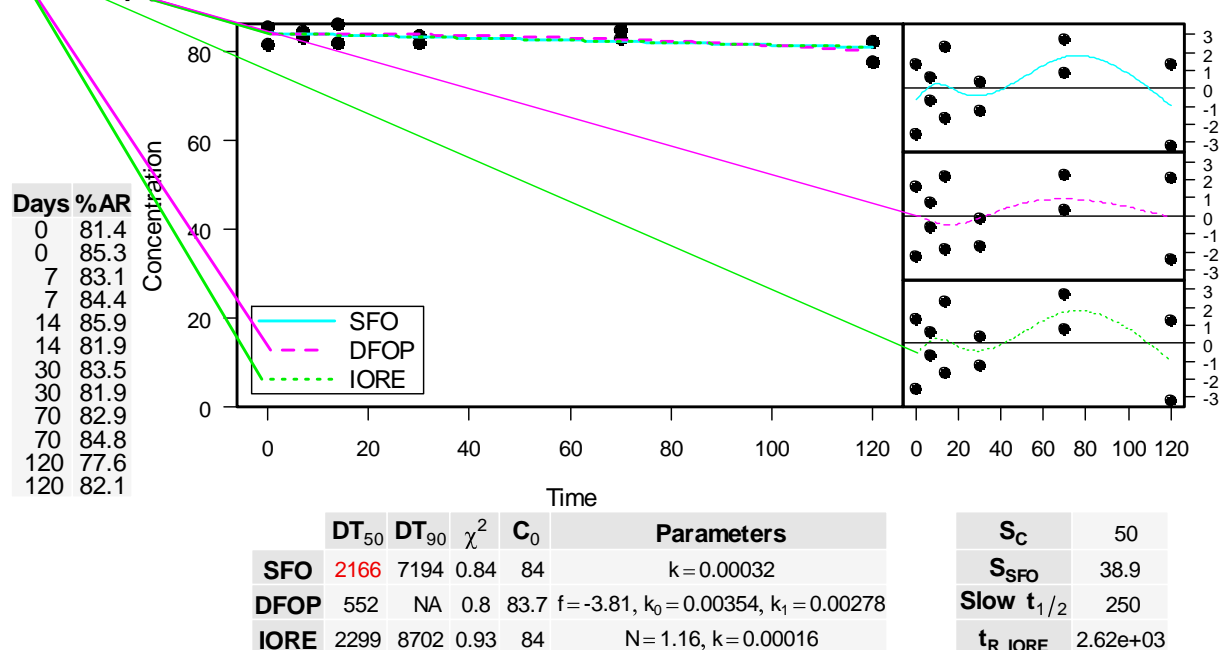
Using Single First Order (SFO) kinetics (KinGUI v 2) with ordinary least-squares fitting, the study author determined dithiopyr (total system) dissipation DT50 values for of 627 days in the DU-L-PF clay loam soil system, 778 days in the Hareby clay loam soil system, and >1,000 days in the silt loam and sandy loam soil systems (pp. 27, 32; Table 15, p. 49).

Dissipation kinetics

Dithiopyr in anaerobic DU-L-PF clay loam soil

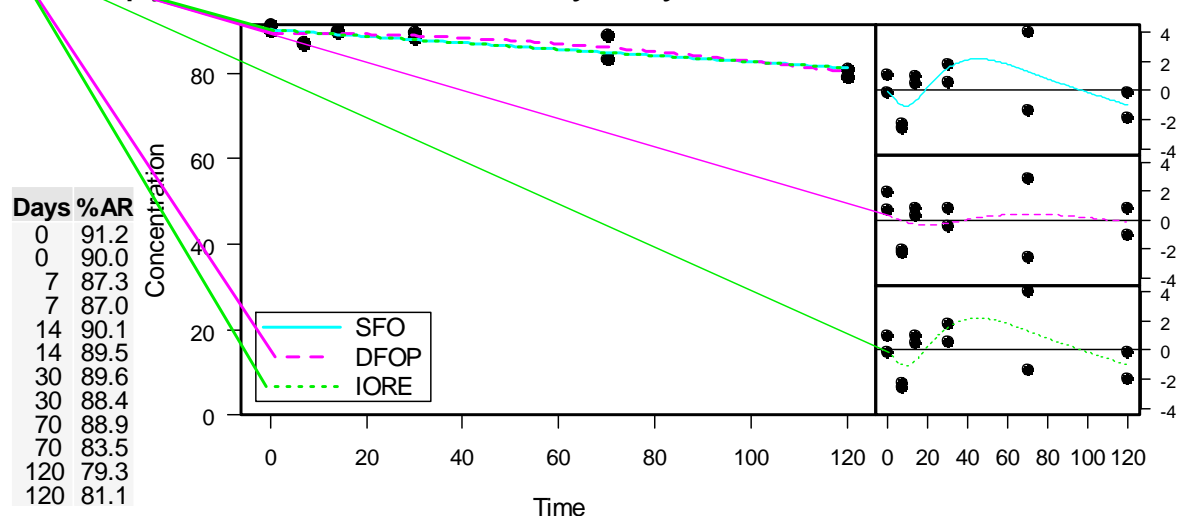


Dithiopyr in anaerobic Iowa silt loam soil



Kinetics models: Single First Order (SFO); Double First Order in Parallel (DFOP), and Indeterminate Order Rate Equation (IORE) in accordance with NAFTA kinetics guidance (USEPA, 2012).

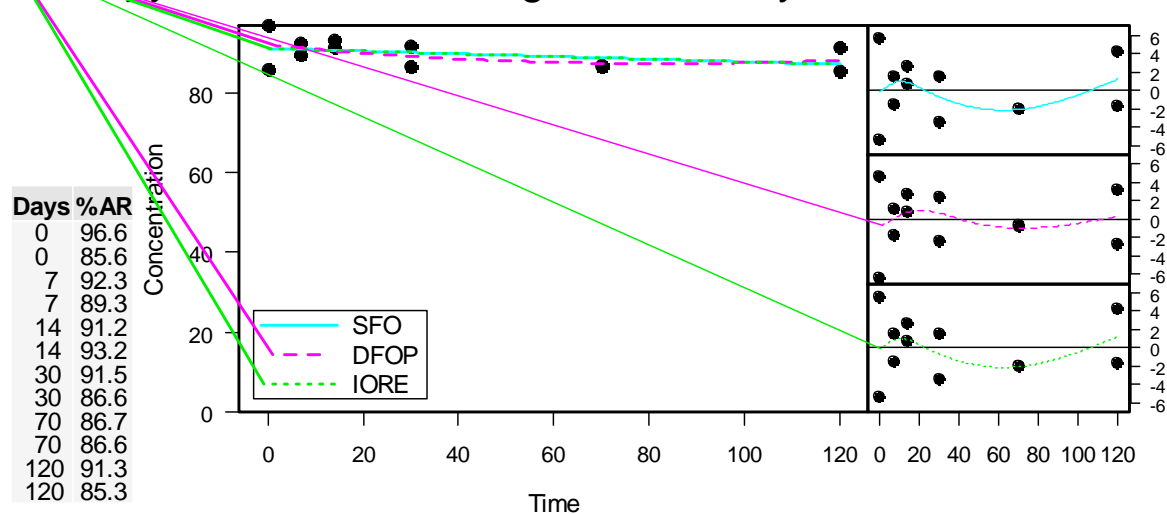
Dithiopyr in anaerobic Hareby clay loam soil



	DT ₅₀	DT ₉₀	χ^2	C ₀	Parameters
SFO	795	2642	1.2	90.2	k = 0.000872
DFOP	365	NA	1.2	89.3	f = -1.97, k ₀ = 0.00586, k ₁ = 0.00384
IORE	907	4378	1.4	90.2	N = 1.42, k = 0.000134

S_C	51.8
S_{SFO}	40
Slow t_{1/2}	181
t_{R IORE}	1.32e+03

Dithiopyr in anaerobic Longwoods sandy loam soil



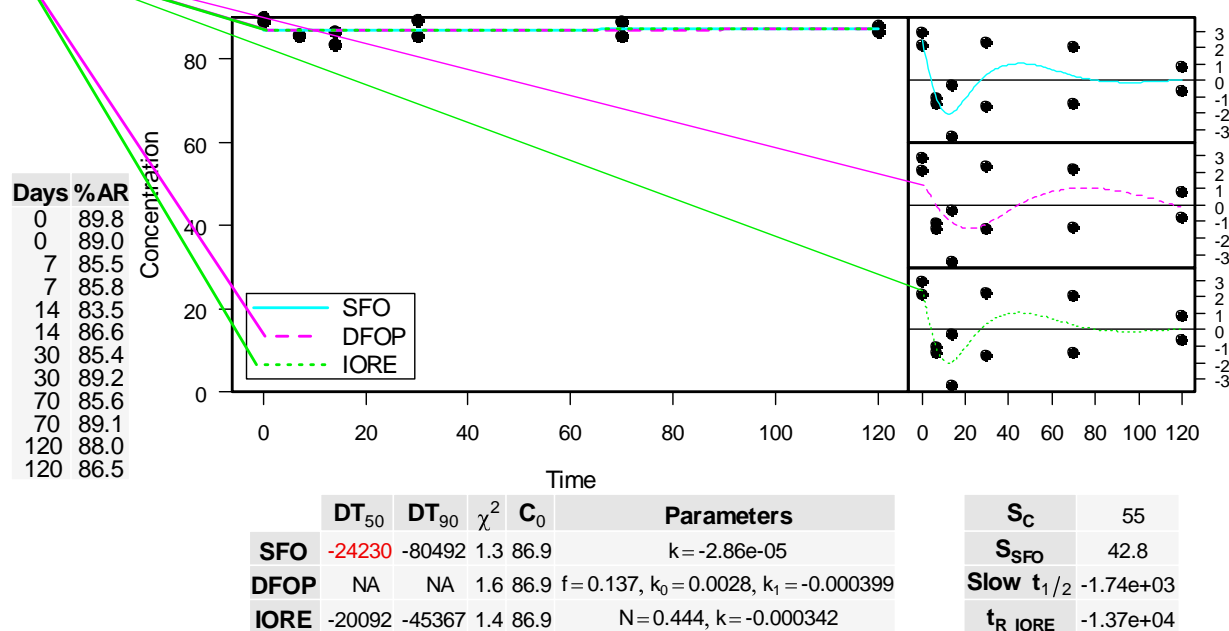
	DT ₅₀	DT ₉₀	χ^2	C ₀	Parameters
SFO	1861	6182	1.1	91	k = 0.000372
DFOP	NA	NA	0.97	92	f = 0.404, k ₀ = 0.00644, k ₁ = -0.00215
IORE	2132	10344	1.2	91	N = 1.43, k = 5.54e-05

S_C	148
S_{SFO}	116
Slow t_{1/2}	-323
t_{R IORE}	3.11e+03

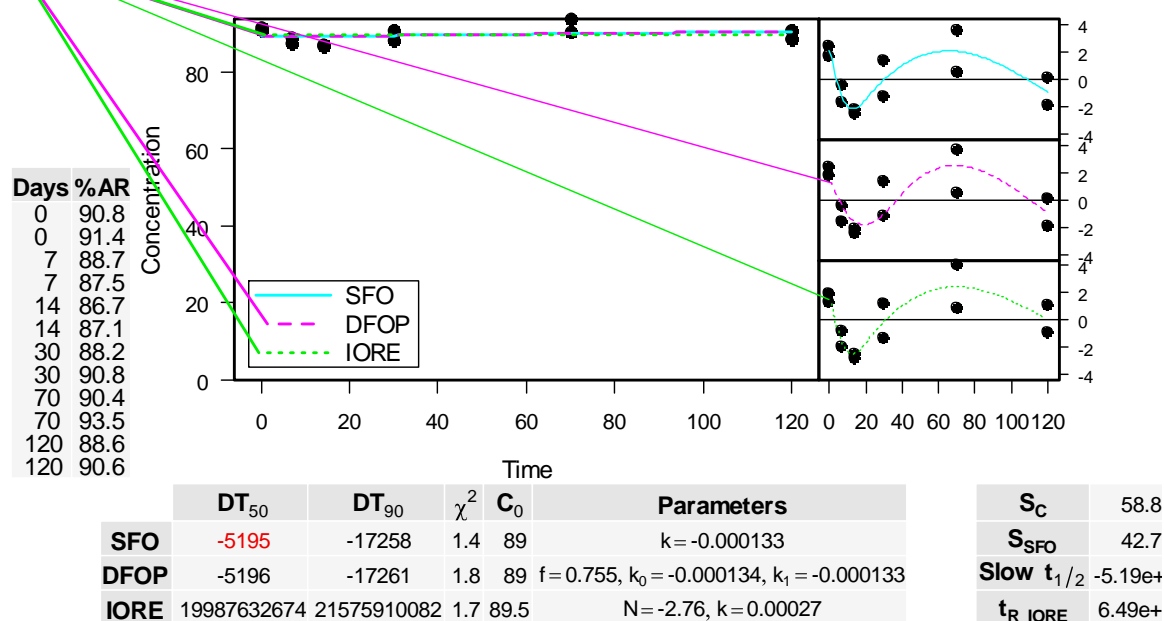
Kinetics models: Single First Order (SFO); Double First Order in Parallel (DFOP), and Indeterminate Order Rate Equation (IORE) in accordance with NAFTA kinetics guidance (USEPA, 2012).

Degradation kinetics (volatile-adjusted)

Volatile-adjusted Dithiopyr in anaerobic DU-L-PF clay loam soil

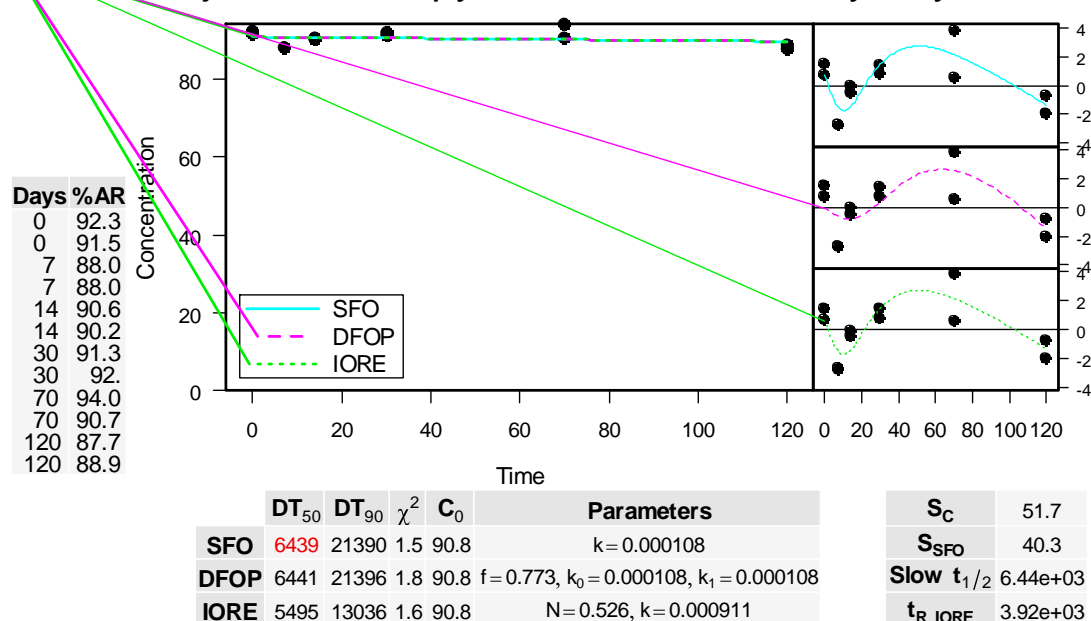


Volatile-adjusted Dithiopyr in anaerobic Iowa silt loam soil

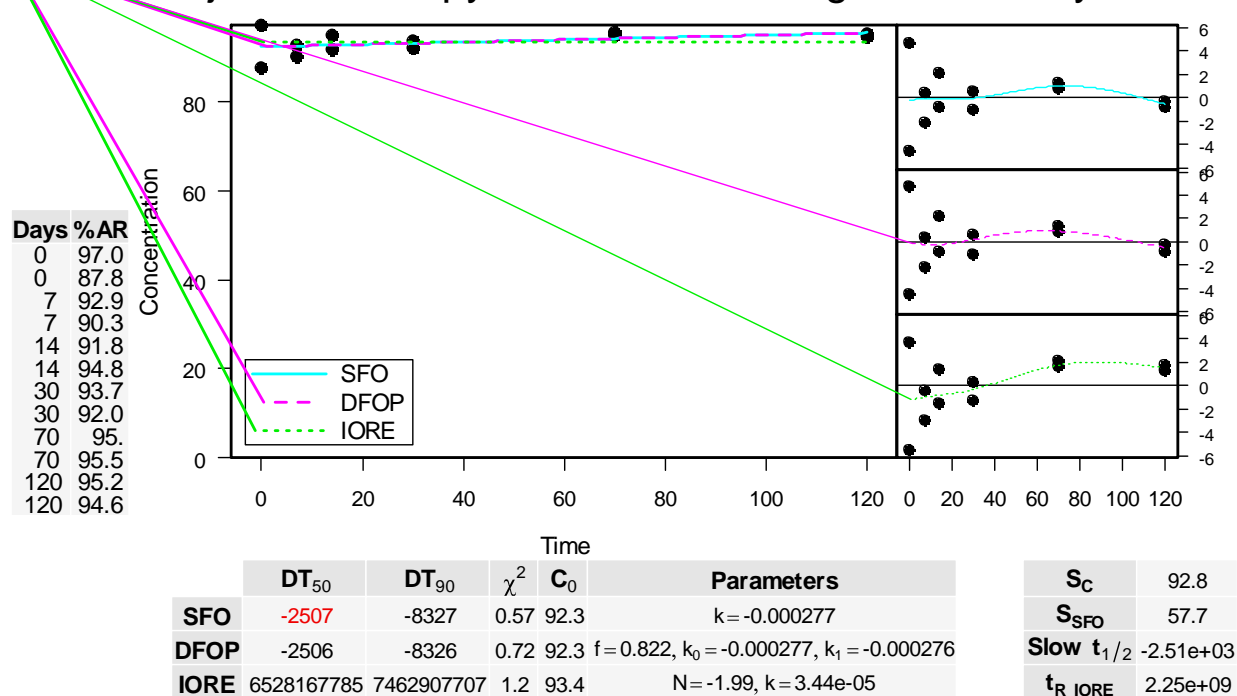


Kinetics models: Single First Order (SFO); Double First Order in Parallel (DFOP), and Indeterminate Order Rate Equation (IORE) in accordance with NAFTA kinetics guidance (USEPA, 2012).

Volatile-adjusted Dithiopyr in anaerobic Hareby clay loam soil



Volatile-adjusted Dithiopyr in anaerobic Longwoods sandy loam soil



Kinetics models: Single First Order (SFO); Double First Order in Parallel (DFOP), and Indeterminate Order Rate Equation (IORE) in accordance with NAFTA kinetics guidance (USEPA, 2012).

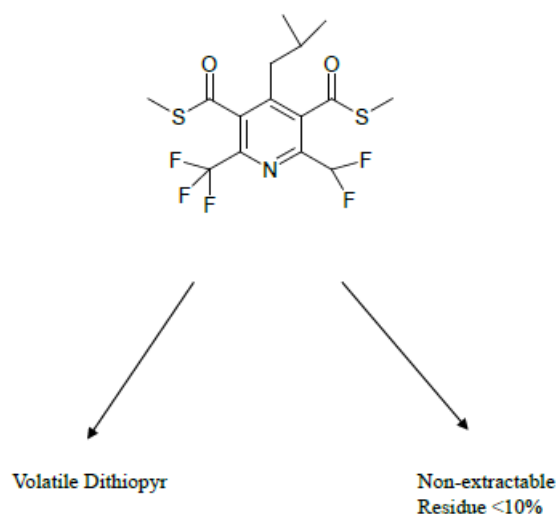
Table 8. Transformation Products of Dithiopyr in Soil.

	Transformation Products	Maximum %AR Observed	Associated Interval (days postflooding)	Final %AR Observed	Final Interval (days postflooding)
North Dakota USA Clay loam soil (DU-L-PF) (20°C, soil pH 6.2)	CP108329	2.44	7	1.52	120
	CP108330	2.44	120	2.44	120
Iowa, USA Silt loam soil (20°C, soil pH 6.1)	CP108329	1.55	30	1.22	120
	CP108330	1.58	120	1.58	120
UK Clay loam soil (Hareby) (20°C, soil pH 7.5)	CP108329	1.57	120	1.57	120
	CP108330	2.79	120	2.79	120
UK Sandy loam soil (20°C, soil pH 7.5)	CP108329	1.40	120	1.40	120
	CP108330	1.66	120	1.66	120

Data obtained from Tables 10-13, pp. 44-47, in the study report.

The soil was flooded at 30 days posttreatment. Day 7 postflooding is equivalent to 37 days posttreatment.

An anaerobic transformation pathway in soil was provided by the study author (Figure 23, p. 74).



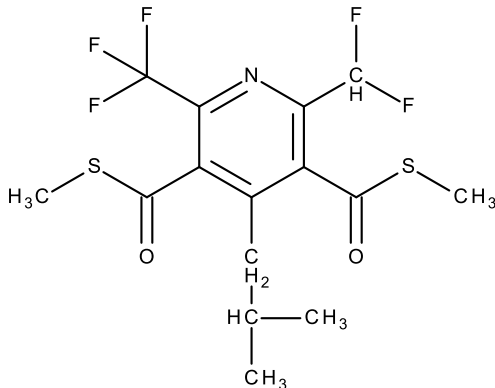
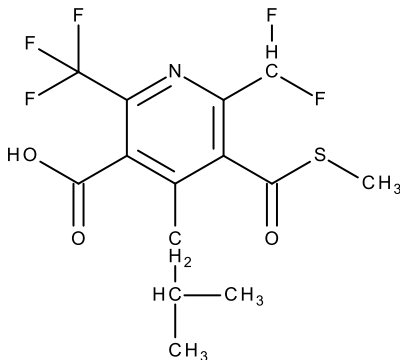
III. STUDY DEFICIENCIES AND REVIEWER'S COMMENTS

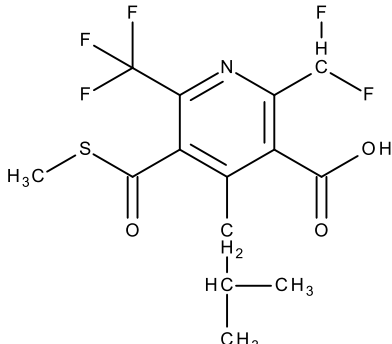
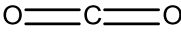
Pesticide use history at the two US soil collection sites was not reported, and it was not confirmed that the soils were free of pesticides prior to use.

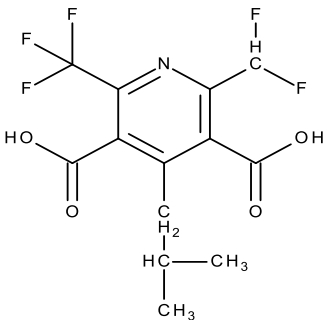
IV. REFERENCES

1. U.S. Environmental Protection Agency. 2008. Fate, Transport and Transformation Test Guidelines, OCSPP 835.4200, Anaerobic Soil Metabolism. Office of Chemical Safety and Pollution Prevention, Washington, DC. EPA 712-C-08-017.
2. U.S. Environmental Protection Agency. 2012. NAFTA Guidance for Evaluating and Calculating Degradation Kinetics in Environmental Studies
(http://www.epa.gov/oppefed1/ecorisk_ders/degradation_kinetics/NAFTA_Degradation_Kinetics.htm.)

DER ATTACHMENT 1. Dithiopyr and Its Environmental Transformation Products. ^A

Code Name/ Synonym	Chemical Name	Chemical Structure	Study Type	MRID	Maximum %AR (day)		Final %AR (study length)
PARENT							
Dithiopyr	<p>IUPAC: S,S'-dimethyl 2-difluoromethyl-4-isobutyl-6-trifluoromethylpyridine-3,5-dicarbothioate</p> <p>CAS: S,S'-dimethyl 2-(difluoromethyl)-4-(2-methylpropyl)-6-(trifluoromethyl)-3,5-pyridinedicarbothioate</p> <p>CAS No.: 97886-45-8</p> <p>Formula: C₁₅H₁₆F₅NO₂S₂</p> <p>MW: 401.4 g/mol</p> <p>SMILES: n1c(C(F)F)c(C(=O)SC)c(CC(C)C)C)c(C(=O)SC)c1C(F)(F)F</p>		835.4200 Anaerobic soil metabolism	50092201	PRT		PRT
MAJOR (>10%) TRANSFORMATION PRODUCTS							
Unextractable residues	NA	NA	835.4200 Anaerobic soil metabolism	50092201	North Dakota Clay loam	10.33% (15 d)	6.11% (150 d)
MINOR (<10%) TRANSFORMATION PRODUCTS							
Mono-acid reverse (CP108329; RH- 131766)	<p>IUPAC: 6-(Difluoromethyl)-4-(2-methylpropyl)-5-(methylthio)carbonyl-2-(trifluoromethyl)-3-pyridinecarboxylic acid</p> <p>Formula: C₁₄H₁₄F₅NO₃S</p> <p>MW: 371.3 g/mol</p> <p>SMILES: CC(C)Cc1c(nc(c1C(=O)O)C(F)(F)F)C(=O)SC</p>		835.4200 Anaerobic soil metabolism	50092201	North Dakota Clay loam	2.44% (37 d)	1.52% (150 d)
					Silt loam	1.55% (60 d)	1.22% (150 d)
					UK Clay loam	1.57% (150 d)	1.57% (150 d)
					Sandy loam	1.40% (150 d)	1.40% (150 d)

Code Name/ Synonym	Chemical Name	Chemical Structure	Study Type	MRID	Maximum %AR (day)		Final %AR (study length)
Mono-acid II (CP108330; RH-131765)	IUPAC: 2-(Difluoromethyl)-4-(2-methylpropyl)-5-(methylthio)carbonyl-6-(trifluoromethyl)-3-pyridinecarboxylic acid Formula: C ₁₄ H ₁₄ F ₅ NO ₃ S MW: 371.3 g/mol SMILES: <chem>CC(C)Cc1c(c(nc(c1C(=O)SC)C(F)(F)F)C(F)F)C(=O)O</chem>		835.4200 Anaerobic soil metabolism	50092201	North Dakota Clay loam	2.44% (150 d)	2.44% (150 d)
					Silt loam	1.58% (150 d)	1.58% (150 d)
					UK Clay loam	2.79% (150 d)	2.79% (150 d)
					Sandy loam	1.66% (150 d)	1.66% (150 d)
Carbon dioxide	IUPAC: Carbon dioxide Formula: CO ₂ MW: 44 g/mol SMILES: C(=O)=O		835.4200 Anaerobic soil metabolism	50092201	North Dakota Clay loam	<0.1% (0-150 d)	<0.1% (150 d)
					Silt loam	<0.1% (0-150 d)	<0.1% (150 d)
					UK Clay loam	<0.1% (0-150 d)	<0.1% (150 d)
					Sandy loam	<0.1% (0-150 d)	<0.1% (150 d)

Code Name/ Synonym	Chemical Name	Chemical Structure	Study Type	MRID	Maximum %AR (day)	Final %AR (study length)
REFERENCE COMPOUNDS NOT IDENTIFIED						
Di-acid (RH-133972)	IUPAC: 2-(Difluoromethyl)-4-isobutyl-6-(trifluoromethyl)pyridine-3,5-dicarboxylic acid Formula: C ₁₃ H ₁₂ F ₅ NO ₄ MW: 341.2 g/mol SMILES: <chem>CC(C)Cc1c(c(nc(c1C(=O)O)C(F)(F)F)C(F)F)C(=O)O</chem>		835.4200 Anaerobic soil metabolism	50092201	NA	NA

^A AR means “applied radioactivity”. MW means “molecular weight”. PRT means “parent”. NA means “not applicable”.

Organic volatiles in the polyurethane foam plugs, which were identified as dithiopyr, were maximums of 13.09% of the applied in the North Dakota clay loam soil system, 11.35% in the silt loam soil system, 8.77% in the UK clay loam soil system and 9.21% in the sandy loam soil system at 120 days postflooding.

Attachment 2: Statistics Spreadsheets and Graphs

Attachment 3: Calculations

Calculations were performed by the reviewer using PestDF, and the following equations.

Single First-Order (SFO) Model

$$C_t = C_0 e^{-kt} \quad (\text{eq. 1})$$

where,

C_t = concentration at time t (%)

C_0 = initial concentration (%)

e = Euler's number (-)

k = SFO rate constant of decline (d^{-1})

t = time (d)

The SFO equation is solved with R kinetics software by adjusting C_0 and k to minimize the objective function (S_{SFO}) shown in equation 9.

$$DT_{50} = \text{natural log}(2)/k \quad (\text{eq. 2})$$

$$DT_{90} = \ln(10)/k \quad (\text{eq. 3})$$

Indeterminate Order Rate Equation (IORE) Model

$$C_t = \left[C_0^{(1-N)} - (1-N)k_{IORE}t \right]^{\frac{1}{1-N}} \quad (\text{eq. 4})$$

where,

N = order of decline rate (-)

k_{IORE} = IORE rate constant of decline (d^{-1})

This equation is solved with R kinetics software by adjusting C_0 , k_{IORE} , and N to minimize the objective function for IORE (S_{IORE}) (See equation 9). Half-lives for the IORE model are calculated using equation 5, which represents a first-order half-life that passes through the DT_{90} of the IORE model. (Traditional DT_{50} and DT_{90} values for the IORE model can be calculated using equations 6 and 7.)

$$t_{IORE} = \frac{\log(2) C_0^{1-N} (1 - 0.1^{(1-N)})}{\log(10) (1-N)k_{IORE}} \quad (\text{eq. 5})$$

$$DT_{50} = \frac{(C_0/2)^{(1-N)} - C_0^{(1-N)}}{k(N-1)} \quad (\text{eq. 6})$$

$$DT_{90} = \frac{(C_0/10)^{(1-N)} - C_0^{(1-N)}}{k(N-1)} \quad (\text{eq. 7})$$

Double First-Order in Parallel (DFOP) Model

$$C_t = C_0 g^{-k_1 t} + C_0 (1 - g)^{-k_2 t} \quad (\text{eq. 8})$$

where,

g = the fraction of C_0 applied to compartment 1 (-)

k_1 = rate constant for compartment 1 (d^{-1})

k_2 = rate constant for compartment 2 (d^{-1})

If $C_0 \times g$ is set equal to a and $C_0(1-g)$ is set equal to c , then the equation can be solved with R kinetics software for a , c , k_1 , and k_2 by minimizing the objective function (S_{DFOP}) as described in equation 9.

DT_{50} and DT_{90} values can be calculated using equations 2 and 3, with k_1 or k_2 in place of k .

Objective Function: SFO, IORE, and DFOP are solved by minimizing the objective function (S_{SFO} , S_{IORE} , or S_{DFOP}).

$$S_{\text{SFO}}, S_{\text{IORE}}, \text{ or } S_{\text{DFOP}} = \sum (C_{\text{model}, t} - C_{d,t})^2 \quad (\text{eq. 9})$$

where,

S_{SFO} , S_{IORE} , or S_{DFOP} = objective function of kinetics model fit ($\%^2$)

n = number of data points (-)

$C_{\text{model}, t}$ = modeled value at time corresponding to $C_{d,t}$ (%)

$C_{d,t}$ = experimental concentration at time t (%)

Critical Value to Determine Whether SFO is an Adequate Kinetics Model

If S_{SFO} is less than S_c , the SFO model is adequate to describe kinetics. If not, the faster of t_{IORE} or the DFOP DT_{50} for compartment 2 should be used.

$$S_c = S_{\text{IORE}} \left(1 + \frac{p}{n-p} F(\alpha, p, n-p) \right) \quad (\text{eq. 10})$$

where,

S_c = the critical value that defines the confidence contours ($\%^2$)

p = number of parameters (3 in this case)

α = the confidence level (0.50 in this case)

$F(\alpha, p, n-p)$ = F distribution with α level of confidence and degrees of freedom p and $n-p$



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